Year-End Summary Report
(Summer 2007 NARC)

TITLE: Nonlinear Interactions of Light with Liquid Crystals
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1 BACKGROUND

Crystals are solids in which the molecules are arranged in clearly defined 3D patterns. *Liquid crystals* are substances whose constituent molecules retain the spatial regularity of solid crystals, but, at the same time, have the freedom of motion of molecules of a conventional liquid.

Common usage of liquid crystals includes household appliances such as microwave ovens, CD players, or thermometers and even wrist watches, but they have an increasingly visible application as the main component in LCD monitors. In fact, the acronym "LCD" stands for *liquid crystal display.*

Liquid crystals can be classified by the type of directional and positional ordering of the constituent molecules into several categories (phases), of which the most common is the *nematic phase.* This is the type used in LCD monitors, and is the object of our study. The molecules of a nematic liquid crystal have a cylindrical shape, and can move randomly. Having one axis longer than the other two, it makes sense to talk about orientation of these molecules, which can be modeled mathematically by a unit vector field

$$\vec{n} = \vec{n}(x_1, x_2, x_3)$$

called *director*. The one defining property of nematics is that in the absence of external factors such as electro-magnetic fields, or temperature fluctuations, the director is roughly *spatially invariant.* That is, the cigar shaped molecules tend to align themselves with their long axis parallel to a preferred direction.

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The orientation of the molecules determines the *optical properties* of the material. This means, for instance, that controlling what is being displayed on an LCD monitor, amounts to controlling the director vector field $\vec{n}$.

The director vector field $\vec{n}$ of a liquid crystal minimizes an energy functional (termed *free energy*) of the form

$$\mathcal{E}(\vec{n}) = \int_\Omega F(\vec{n}, \nabla\vec{n})\, d\omega \tag{1}$$

subject to the constraint

$$|\vec{n}| = 1$$

In the absence of an electric or magnetic field, the free energy *density* is given by

$$F(\vec{n}, \nabla\vec{n}) = \underbrace{K_1|\nabla\cdot\vec{n}|^2}_{splay} + \underbrace{K_2|\vec{n}\cdot(\nabla\times\vec{n})|^2}_{twist} + \underbrace{K_3|\vec{n}\times(\nabla\times\vec{n})|^2}_{bend} \tag{2}$$

In any medium (not only liquid crystals), an electric field E is accompanied by a magnetic field H, related by a pair of equations (*Maxwell's equations*):

$$\begin{aligned} -\partial_t B &= \nabla\times E \\ \partial_t D &= \nabla\times H \end{aligned} \tag{3}$$

in which D is the *electric displacement* field, B is the *magnetic inductance* field, each defined by the following two *constituent equations*:

$$D = \epsilon E + P \tag{4}$$

$$B = \mu H + M \tag{5}$$

In equations (4) and (5), P and M are the electric and the magnetic polarizations, respectively. In general, P depends on E and M depends on H. The *electric permittivity* ϵ and the *magnetic permeability* μ are, in general, functions which may depend on the position vector and on the optical and magnetic properties of the medium, respectively.

It has been shown (see e.g., [1]), that in the case of a nematic liquid crystal, the electric displacement is equal to

$$D = \epsilon E + \Delta\epsilon(\vec{n} \cdot E)\vec{n} \tag{6}$$

Moreover, an electric field E applied to an electric field modifies the infinitesimal energy $F(\vec{n}, \nabla\vec{n})$ by the amount

$$F_E = -\frac{\Delta\epsilon}{2}(\vec{n} \cdot E)^2 \tag{7}$$

and similarly, a magnetic field has an infinitesimal contribution

$$F_H = -\frac{\Delta\chi}{2}(\vec{n} \cdot H)^2 \tag{8}$$

Thus, the presence of an electric field and a magnetic field produces a free energy density given by

$$\begin{aligned} F(\vec{n}, \nabla\vec{n}) = \underbrace{K_1|\nabla \cdot \vec{n}|^2}_{splay} + \underbrace{K_2|\vec{n} \cdot (\nabla \times \vec{n})|^2}_{twist} + \underbrace{K_3|\vec{n} \times (\nabla \times \vec{n})|^2}_{bend} \\ - \underbrace{\frac{\Delta\epsilon}{2}(\vec{n} \cdot E)^2}_{electric} - \underbrace{\frac{\Delta\chi}{2}(\vec{n} \cdot H)^2}_{magnetic} \end{aligned} \tag{9}$$

2 OBJECTIVE

The objective is to study light propagation through a nematic liquid crystal. This includes modeling of the phenomenon (by finding the relevant quantities and the equations that these quantities satisfy), and trying to solve the resulting equations.

In general, when solving differential equations, one must prove:

- existence of solutions
- uniqueness of the solutions
- regularity

In addition, a numerical implementation of the solutions (if they exist) is desirable.

2.1 Light propagation through liquid crystals: Proposed model

Light is *simultaneously* both an electric field an a magnetic field (E and H, respectively). Its propagation through any medium is completely described by Maxwell's equations (3), and depends on the optical properties of that medium. In the case of nematic liquid crystals, the most important factor is the orientation $\vec{n}$ of the constituent molecules, so definitely E and H depend on $\vec{n}$.

In a linear medium, the electric polarization P and the magnetic polarization M are both zero, by definition. See equations (4), (5) and especially (6). Consequently, $F_E = 0$. Similarly, $F_H = 0$. That is, light passing through a linear medium does not change the director vector field $\vec{n}$. To see how light propagates through the crystal, Maxwell's equations must be solved irrespective of the free energy density (2), by assuming that $\vec{n}$ is given (as an equilibrium state of the free energy), and that it is independent of E and H (but not the other way around).

In the case of a non-linear medium, a powerful polarized light *can* modify the molecular structure of the crystal, due to the non-zero polarization, and this is reflected by equations (6), (7) and (8). Maxwell's equations contain $\vec{n}$ explicitly and the free energy density (9) contains at least one of E or H. Therefore, $\vec{n}$, E and H are *coupled* (depend on each other), and must be determined simultaneously.

We model light propagation through a liquid crystal by the following minimization problem:

Problem 2.1 *Minimize*

$$\mathcal{E}(\vec{n}, \nabla\vec{n}, E, H) = \int_\Omega \Big(K_1|\nabla\cdot\vec{n}|^2 + K_2|\vec{n}\cdot(\nabla\times\vec{n})|^2 + K_3|\vec{n}\times(\nabla\times\vec{n})|^2 - \frac{\Delta\epsilon}{2}(\vec{n}\cdot E)^2 - \frac{\Delta\chi}{2}(\vec{n}\cdot H)^2 \Big) d\omega$$

subject to

$$\begin{aligned} -\partial_t B &= \nabla\times E \\ \partial_t D &= \nabla\times H \end{aligned}$$

$$D = \epsilon E + P$$
$$B = \mu H + M$$

and

$$|\vec{n}| = 1.$$

Remark 2.1 The contributions F_E and F_H of an electromagnetic field to the free density $F(\vec{n}, \nabla\vec{n})$ were derived elsewhere by other researchers. The addition of F_E and F_H to F assumed that E and H did not depend on $\vec{n}$, nor of each other. Minimization of the free energy (1) was still performed after $\vec{n}$ alone.

Neglecting the coupling of E and H via Maxwell's equations, as well as their dependence on $\vec{n}$ is no longer reasonable in the case of light passing through a liquid crystal, because Maxwell's equations are the very equations that describe the propagation of light.

In our model, the free energy $\mathcal{E}$ is minimized after $\vec{n}$, E and H, and E, H and $\vec{n}$ are assumed to depend (a priori) on each other.

3 METHODS and RESULTS

3.1 The Euler-Lagrange equations

One first step towards finding a solution is computation of the Euler-Lagrange equations for the functional $\mathcal{E}$, which can be done using standard methods from the *calculus of variations* [2, 3]. In the absence of any constraints, for *any* functional defined as in (1), these equations take the form

$$\sum_{\beta=1}^{3} \frac{\partial}{\partial x_\beta}\Big(\frac{\partial F}{\partial(\partial_\beta n_\alpha)}\Big) - \frac{\partial F}{\partial n_\alpha} = 0. \tag{10}$$

The system (10) represents the *Euler-Lagrange* equations of E, and involves $\vec{n}$ and its derivatives. We computed explicitly this system for F given by equation (2). We state the result below.

3.2 Derivation of model equations

First, we study the propagation of light in a nematic liquid crystal in the presence of an electric field E. We derive a system of coupled equations for the reorientaion of the liquid crystal director $\vec{n}$.

Consider the time harmonic Maxwell's equations (time dependence $e^{i\omega t}$. The electric field E has the form

$$E(x,t) = E(x)e^{i\omega t} + \bar{E}(x)e^{-i\omega t}.$$

Assume that the light wave propagates normally to the liquid-crystal medium and that the initial orientation of the director is along z and that the director can change its direction in the (x, z) plane and, therefore, we write the vector components of the director in the form

$$\vec{n} =< \sin\phi(z), 0, \cos\phi(z) > .$$

Then using this form of the director $\vec{n}$, the free energy density can be derived as

$$F(\vec{n}, \nabla\vec{n}) = (K\sin^2\phi + K\cos^2\phi)(\frac{d\phi}{dz})^2.$$

We also assume that dielectric coefficient ϵ is of the form $\epsilon_{ij} = \epsilon_\perp\delta_{ij} + \epsilon_a n_i n_j$, where $\epsilon_a = \epsilon_\| - \epsilon_\perp$, and $\epsilon_\|, \epsilon_\perp$, are the liquid crystal dielectric constants at the director parallel and perpendicular to the electric field, and $i, j = 1, 2, 3$. Hence the dielectric coefficient ϵ becomes

$$\epsilon = \begin{pmatrix} \epsilon_\perp + \epsilon_a\sin^2\phi & 0 & \epsilon_a\sin\phi\cos\phi \\ 0 & \epsilon_\perp & 0 \\ \epsilon_a\sin\phi\cos\phi & 0 & \epsilon_\perp + \epsilon_a\cos^2\phi \end{pmatrix},$$

and the electric contribution to the total energy can be written as

$$F_E = \epsilon_a[\sin^2\phi|E_1|^2 + \cos^2|E_3| + \sin\phi\cos\phi(E_1\bar{E}_3 + E_3\bar{E}_1) - \epsilon_\perp|E|^2].$$

3.3 Results

Minimizing the free energy with respect to the director $\vec{n}$ (the angle ϕ), using the Euler Langrange equations, we get the following equation for the director

$$K\frac{d^2\phi}{dz^2} + \frac{\epsilon_a\epsilon_\perp(\epsilon_a + \epsilon_\perp|E|^2\sin 2\phi}{(\epsilon_\perp + \epsilon_a\cos^2\phi)^2} = 0 \tag{11}$$

From the Maxwell's equations, we obtain the following equation for the electric field $E =< E_1(z), 0, E_3(z) >$.

$$\frac{d^2E_1}{dz^2} + \omega^2\mu(\epsilon_\perp + \epsilon_a\sin^2\phi E_1 + \epsilon_a\sin\phi\cos\phi E_3) = 0, \tag{12}$$

$$\frac{d^2E_3}{dz^2} + \omega^2\mu(\epsilon_a \sin\phi\cos\phi E_1 + \epsilon_\perp + \epsilon_a \cos^2\phi E_3) = 0. \tag{13}$$

We now solve numerically the coupled nonlinear equations (11)-(13), for $0 \leq z \leq L$. We use the boundary condition $\phi(0) = \phi(L) = 0$. We also assume the electic field is given as the sum of the incident end reflected waves for $z \leq 0$ and the outgoing waves for $z \geq L$,

$$E = \left\{ \begin{array}{l} E_{inc}e^{ikz} + E_{ref}e^{-ikz}, z \leq 0 \\ E_{out}e^{ikz}, z \geq L \end{array} \right) .$$

This numerical implementation is work in progress.

References

[1] J. De Gennes, P.G.and Prost. *The Physics of Liquid Crystals.* Oxford University Press, second edition, 1998.

[2] C. Fox. *An Introduction to the Calculus of Variations.* Dover Publications Inc., 1987.

[3] I.M. Gelfand and S.V. Fomin. *Calculus of Variations.* DOver Publications Inc, 2000.

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